

Instabilities at $[110]$ Surfaces of $d_{x^2-y^2}$ Superconductors

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We compare different scenarios for the low temperature splitting of the zero-energy peak in the local density of states at (110) surfaces of $d_{x^2-y^2}$ -wave superconductors, observed by Covington et al. (Phys.Rev.Lett. **79** (1997), 277). Using a tight binding model in the Bogolyubov-de Gennes treatment we find a surface phase transition towards a time-reversal symmetry breaking surface state carrying spontaneous currents and an $s + id$ -wave state. Alternatively, we show that electron correlation leads to a surface phase transition towards a magnetic state corresponding to a local spin density wave state.

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A large number of experiments have established that the Cooper pair wavefunction has $d_{x^2-y^2}$ -wave symmetry in high-temperature superconductors. Decisive information came from probes which are sensitive to the internal phase structure of the pair wavefunction. Besides experiments based on the Josephson effect [1] also the surface Andreev bound states (ABS) [2] observable in quasiparticle tunneling can be counted among the strongest experimental tests of this type. For a superconductor with pure $d_{x^2-y^2}$ symmetry these ABS should be most pronounced at $[110]$ surfaces and lie exactly at the Fermi energy (zero energy). They lead to a rather sharp zero-bias anomaly in the I-V tunneling characteristics which reflects the surface quasiparticle density of states (DOS) [3]. In addition low temperature anomalies in the penetration depth have been interpreted as evidence for the existence of the zero-energy ABS [4]. An interesting twist in the view of the ABS occurred when Covington et al. [5] observed the spontaneous split of the single zero-energy peak (ZEP) into two peaks at finite voltage equivalent to an energy of approximately 10% of the superconducting gap below $T = 7K$. Fogelström et al. [6] interpreted this in terms of a spontaneous violation of time-reversal symmetry breaking (TRSB) by the admixture of a sub-dominant s -wave component close to the surface. The split ABS is the result of the opening of a small gap in the quasiparticle spectrum at the surface and can be interpreted as a Fermi surface (FS) instability. [7,8] TRSB is not the only way to shift the ZEP to finite energies. Many local FS instabilities could yield the same effect and the one with the largest energy gain, i.e. the highest critical temperature, would finally govern the surface state. In this letter we discuss the instability due to correlation effects among the quasiparticles. The zero-energy ABS consists of degenerate states with a charge current running parallel to the surface (in-plane) in both directions (the *directional degeneracy*) and with both spin up and down (the *spin degeneracy*). The TRSB state lifts the directional degeneracy of charge currents by admixing a subdominant s -

wave component to the d -wave pairing state and a spontaneous finite current appears. [7] On the other hand, the spin degeneracy can be lifted yielding a spin density wave-like state at the surface, although magnetic ordering is absent in the bulk. [10] This instability is driven by the repulsive electron-electron interaction responsible for the strong antiferromagnetic spin fluctuations in the underdoped region of high-temperature superconductors. From this point of view the magnetic instability represents an equally probable way to lift the degeneracy of the zero-energy states.

In the following we analyze the properties of $[110]$ -oriented surface of the $d_{x^2-y^2}$ -wave superconductor on a square lattice forming a strip of finite width (infinitely long along $[1,-1,0]$ -direction) such that we have two surfaces. The translationally invariant direction is denoted by the y -axis and the surface normal direction by the x -axis (Fig.1). We describe this system by a tight-binding model with nearest (t) and next-nearest (t') neighbor hopping, and include an onsite repulsive and a spin-dependent nearest neighbor interaction. The latter generates the superconducting state while the former introduces rather magnetic correlations. The corresponding Hamiltonian has the form

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle \mathbf{x}, \mathbf{x}' \rangle, s} c_{\mathbf{x}s}^\dagger c_{\mathbf{x}'s} - t' \sum_{\langle \mathbf{x}, \mathbf{x}' \rangle', s} c_{\mathbf{x}s}^\dagger c_{\mathbf{x}'s} \\ & + J \sum_{\langle \mathbf{x}, \mathbf{x}' \rangle} \mathbf{S}_{\mathbf{x}} \cdot \mathbf{S}_{\mathbf{x}'} + U \sum_{\mathbf{x}} n_{\mathbf{x}\uparrow} n_{\mathbf{x}\downarrow}. \end{aligned} \quad (1)$$

The interaction terms are decoupled by meanfields involving the onsite charge $n(\mathbf{x}) = \sum_s \langle c_{\mathbf{x}s}^\dagger c_{\mathbf{x}s} \rangle$, the onsite magnetic moment $m(\mathbf{x}) = \sum_s \mathbf{s} \langle c_{\mathbf{x}s}^\dagger c_{\mathbf{x}s} \rangle$ and the pairing on nearest neighbor sites $\Delta_{s,s'}(\mathbf{x}, \mathbf{x}') = \langle c_{\mathbf{x}s} c_{\mathbf{x}'s'} \rangle$ which include both $S = 0$ and $S = 1$ pairing. However, spin-triplet pairing is suppressed due the repulsive nature of the interaction in that channel, if we chose $J > 0$. It is sufficient for our analysis to include pairing meanfields $\Delta_{s,-s}(\mathbf{x}, \mathbf{x}')$ on the bonds. This yields basically four types of gap functions, two with singlet (s - and d -wave) and two with spin-triplet (p_x - and p_y -wave with $S_z = 0$) pairing. Among these we find the

$d_{x^2-y^2}$ -wave (or d_{xy} in our rotated coordinates) state as dominant bulk phase. An on-site s -wave without nodes is excluded here, instead we obtain an extended s -wave state. In Fig.1 we symbolize the corresponding gap functions of these three relevant pairing states in momentum space. All the position dependent mean-fields are then determined selfconsistently together with current densities and the vector potential solving the corresponding Bogolyubov-deGennes equations. For the solution of the Maxwell equation we impose the boundary conditions of zero magnetic field at the surface and vanishing vector potential in the bulk. We consider two typical cases for the band structure: (1) band filling approximately 60% and $t' = 0$, where the FS has nearly circular shape (*regular FS*); (2) band filling nearly 85% and $t' = -0.3t$ with the FS close to van Hove singularities (VHS) at $(\pi, 0)$ and $(0, \pi)$ (*singular FS*). The latter case represents the situation in underdoped, the former rather in overdoped region of the cuprate phase diagram.

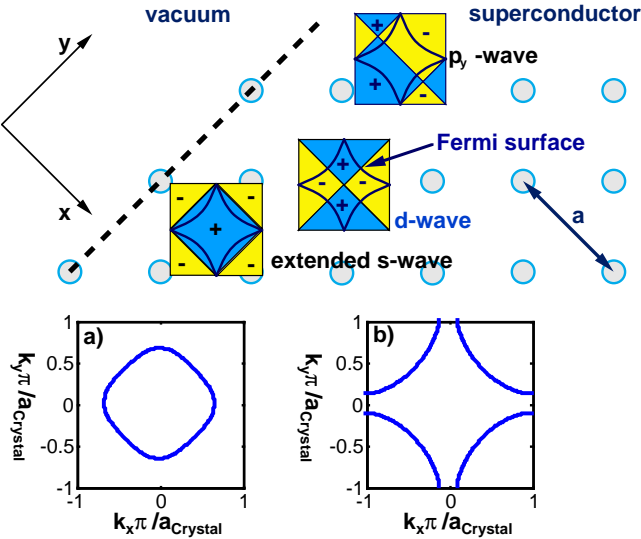


FIG. 1. Geometry and coordinate system of the [110] boundary. The symmetries of the relevant gap functions are symbolized by the + and - regions in the Brillouin zones. a) Fermi surface for the *regular FS* parameters given in the text. b) Fermi surface for *singular FS* parameters. In our notation $a = \sqrt{2}a_{\text{Crystal}}$

First we consider the *regular FS*. The instability in the charge channel can be examined by setting $U = 0$. With the pairing symmetry restricted to the $d_{x^2-y^2}$ -wave channel, the only instability possible is by generating a spontaneous current running along the surface. The mechanism can be understood in the following way. Assume a vector potential $A_y(x)$ along the surface. This will shift the ABS carrying charge in one direction to negative energies, and, thus, creating a paramagnetic surface current which decays into the bulk on the distance of the superconducting coherence length ξ . The energy gain

$-\int dx j_y(x) A_y(x)$ through the surface currents is basically $\propto A_y$, while the energy costs from the required Meissner screening currents are only $\propto A_y^2$. This then leads to a minimum of the total energy for a certain finite $A_y(x)$. We will call this TRSB state the spontaneous surface current (SSC) state. The spatial dependence of the vector potential $A_y(x)$, diamagnetic and paramagnetic current densities and the d -wave gap function are shown in Fig.2. From quasi-classical calculations [9] one expects a critical temperature T_c^{SSC} of the order $(\xi/\lambda)T_c^d$, i.e. rather small for a typical high- T_c superconductor. Our numerical results show $T_c^{\text{SSC}} = 0.006t$ or $T_c^{\text{SSC}}/T_c^d \approx \frac{1}{2}\xi/\lambda$. This low transition temperature indicates that the split of the ABS levels is rather small and barely visible in the surface DOS. We conclude that this surface instability is a poor candidate in order to explain the experimental observations.

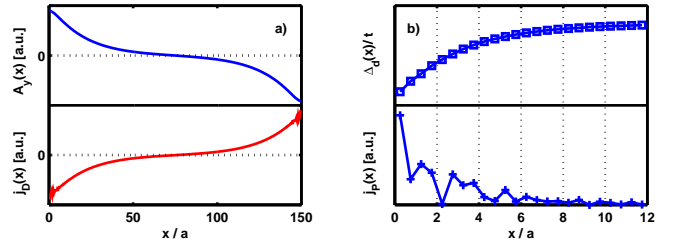


FIG. 2. Spontaneous surface current state: a): Vector potential A_y and diamagnetic Meissner current density j_D . b): d -wave gap function Δ_d and the paramagnetic surface current density j_P carried by the Andreev bound states (system width $150a$, $\mu = -t$, $t' = 0$, $\lambda \approx 18a$ and $T = 0.001t$ yielding critical temperatures $T_c^{\text{SSC}} = 0.006t$ and $T_c^d = 0.11t$).

Now we include a finite s -wave component with a relative phase of $\pm\pi/2$ with respect to the d -wave gap ($s \pm id$). This phase is chosen to maximize the condensation energy of the surface state. Since this TRSB s -wave admixture also lifts the charge degeneracy by changing the Andreev reflection properties for the states with left and right going charge currents, it leads naturally to a net surface current. In the presence of a finite attractive s -wave coupling this will lead to an additional contribution in the gap function increasing the energy gain and resulting in a wider splitting of the ZEP. As a consequence the critical temperature for this $s+id$ state is higher than for the SSC state without s -component. Spatial and temperature dependence of s -admixture and vector potential are shown in Fig.3. For our choice of parameters, the split in the surface DOS has similar size relative to the bulk gap value as in the experiment.

The onsite Coulomb repulsion U itself does not suppress the extended s -wave admixture induced at the boundary, but it can generate a finite magnetization $m(\mathbf{x})$ which then competes with this superconducting state.

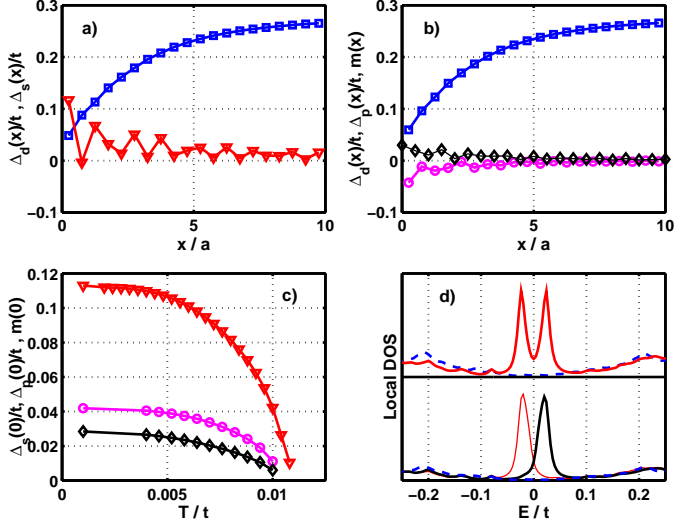


FIG. 3. Regular FS scenario (i.e. $t' = 0$, $J = 2t$, $\mu = -t$ and $T_c^d = 0.11t$): a) d -wave gap (squares) and TRSB s -wave admixture (triangles) at $T = 0.001t$ for $U = 0$. b) d -wave gap, magnetization (diamonds) and TRSB p -wave admixture (circles) at $T = 0.001t$ for $U = t$. c): Temperature dependence of the s -wave gap function, p -wave gap function and magnetization on the first site. d) upper panel: Local DOS in the $s + id$ state at the surface (solid line) and in the bulk (dashed line); lower panel: Local DOS in the magnetic surface state at the surface (solid lines, spin-up and spin-down DOS separate) and in the bulk (dashed line).

If we look for a surface state with finite magnetization for the *regular FS*, we find indeed that already for $U = t$ its critical temperature is comparable to that of the $s + id$ -wave state. For the *regular FS* parameters the weak spin polarization (less than 3%) is ferrimagnetic and decays into the bulk on the scale of the superconducting coherence length. It is accompanied by a TRSB spin-triplet p -wave admixture. The p_y -wave component is induced directly by the d -wave state because the spin rotational symmetry is broken such that the total spin of the pair is not a good quantum number anymore. The p_x -wave component does not appear, since it is odd with respect to specular reflection at the surface and is suppressed by pair breaking. Note that neither the magnetization nor the p -wave admixture lift the directional degeneracy. Therefore the magnetic surface state does not generate charge or spin surface currents. The split in the surface DOS by the magnetic state is shown in Fig.3. As a consequence of the lifted spin degeneracy of the ABS the surface DOS is different for spin-up (with respect to the magnetization axis) and spin-down electrons, a property which could be tested by spin-polarized quasiparticle tunneling.

In Fig.5 we show the U -dependence of the critical temperatures for the two different surface instabilities. Already U slightly larger than t yields a higher T_c for the

magnetic surface state. In a narrow range of parameters the coexistence of $s + id$ and magnetic surface state is possible.

Next we consider the case of the *singular FS* close to the VHS by choosing $t' = -0.3t$ and $\mu = -t$. In order to obtain approximately the same value for the d -wave gap magnitude as in the previous case, we take $J = 1.2t$. Due to the VHS a large part of the low-energy quasiparticles come from the k -space regions around the $(\pi, 0)$ and $(0, \pi)$ points (in crystal coordinates). Since the wave function of the ABS is $\propto \sin k_{Fx}x$ and $k_{Fx} \approx \pi/a$ for most quasiparticles all quantities which live on the bonds and involve products of wave functions on neighboring sites (at distance $a/2$) oscillate like $\sin 2k_{Fx}x$. This also holds for the current carried by the bound states and the s -wave admixture at the surface. As a consequence, the surface currents carried by the ABS are nearly canceled and we do not find a transition towards a pure d -wave SSC state down to very low temperatures. This is in contrast to the results for the regular FS, that resemble those from quasi-classical theory which is insensitive to effects on such a microscopic length scale. Even if we admit a finite s -wave coupling the critical temperature for the s admixture is drastically reduced compared with the previous case ($T_c^s \approx 0.005t$) (Fig.4). The main reason for the small T_c^s is that the FS lies close to the node lines of the extended s -wave gap. Due to the smaller s -wave admixture the split in the ZEP for the $s + id$ -wave state is rather weak (see Fig.4 d)). Our results are in qualitative agreement with the results of Tanuma et al. [11] who use a $t - J$ model in Gutzwiller approximation at comparable band filling.

For finite Coulomb repulsion $U = t$ we again find a magnetic surface state. The VHS enhance correlations with the wavevector close to (π, π) so that the magnetization resembles a spin density wave with period a decaying towards the bulk region (see Fig.4 b)). The induced p_y gap component also exhibits $2k_F$ oscillations. We obtain a sizable split in the surface DOS, the spin-resolved density of states is shown in the lower panel of Fig.4. We find also additional bound states at higher positive energies. This is apparently an effect of the FS, the vicinity to the VHS is responsible for the strong electron-hole asymmetry. However these bound states exist in the entire d -wave phase and are therefore not related to the low temperature surface phase transitions. We would like to remark here: (1) the magnetization approaches the ideal staggered magnetization with period a when we choose $t' = 0$ and, additionally, stay close to half filling; (2) the chosen values $U = t$ and $t' = -0.3t$ are insufficient to establish a Neel state in the bulk in the absence of superconductivity. However, the rearrangement of the ABS provides a mechanism to stabilize the magnetic surface state.

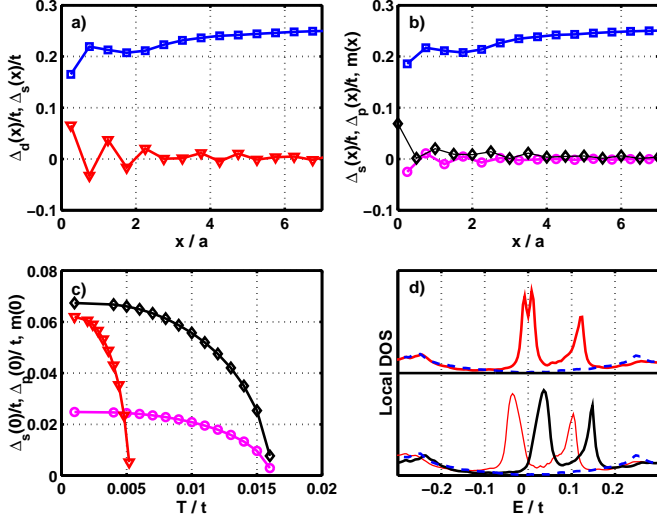


FIG. 4. Singular FS scenario (i.e. $t' = -0.3t$, $J = 1.2t$, $\mu = -t$ and $T_c^d = 0.12t$): a) d -wave gap (squares) and TRSB s -wave admixture (triangles) at $T = 0.001t$ for $U = 0$. b) d -wave gap, magnetization (diamonds) and TRSB p -wave admixture (circles) at $T = 0.001t$ for $U = t$. c) Temperature dependence of the s -wave gap function, p -wave gap function and magnetization on the first site. d) upper panel: Local DOS in the $s + id$ state at the surface (solid line) and in the bulk (dashed line); lower panel: Local DOS in the magnetic surface state at the surface (solid lines, spin-up and spin-down DOS separate) and in the bulk (dashed line).

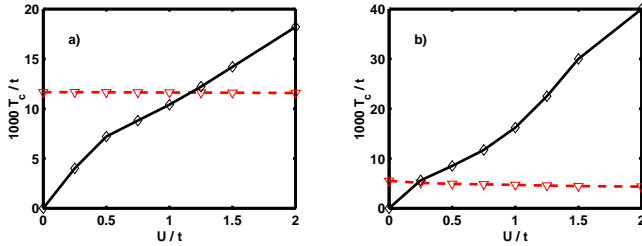


FIG. 5. U -dependence of the critical temperature for the $s + id$ -wave (dashed line) and the magnetic surface state (solid line) for the regular FS (a)) and the singular FS scenario (b)).

For the *singular FS* the critical temperature T_c^m for the magnetic surface state easily exceeds T_c^s for the $s + id$ -wave state (see Fig. 4 c) and Fig. 5), so that our results suggest that the magnetic surface state is the most stable state in the considered frame of possibilities. However an external magnetic field creating a Doppler shift for the quasiparticles and therefore again lifting the charge degeneracy of the ABS would support the $s + id$ -wave state in the competition with the seemingly quite robust magnetic surface state. Note that the charge coupling corresponds to a considerably higher energy scale than the Zeeman coupling which is negligible in this case. This could induce a transition between these two surface states

as the external field is increased. We also refer the reader to a recent preprint by Hu and Yan [12], who discuss possible giant magnetic moments due to the split surface states.

In summary, we have considered different mechanisms to explain the observed low temperature splitting of the ZEP at [110] surfaces of d -wave superconductors. On the one hand, we find that a TRSB superconducting state leads to this effect which is induced by the Doppler shift of a spontaneous surface current [9] or by the local admixture of an s -wave component ($s + id$) [6,8]. On the other hand, electron correlation effects lead to a magnetic instability related to the antiferromagnetic state. Naturally, the latter is more stable in the underdoped regime represented in our case by the model with a singular FS. The former has a better chance to be realized in the overdoped region (regular FS) where the antiferromagnetic spin fluctuations are sufficiently reduced. The experimental distinction between the two states is possible by spin-polarized tunneling as the magnetic state leads to a splitting of the surface DOS for up and down spin.

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